Heat conduction in the diatomic Toda lattice revisited

Takahiro Hatano

Department of Pure and Applied Sciences, University of Tokyo, Komaba, Tokyo 153-0041, Japan
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The problem of the diverging thermal conductivity in one-dimensional (1-D) lattices is considered. By numerical simulations, it is confirmed that the thermal conductivity of the diatomic Toda lattice diverges, which is opposite to what one has believed before. Also the diverging exponent is found to be almost the same as the FPU chain. It is reconfirmed that the diverging thermal conductivity is universal in 1-D systems where the total momentum preserves.

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Heat conduction in one-dimensional lattice is rather an old problem. Many authors have investigated the property of thermal conductivity to understand what ingredients are essential to the standing of a macroscopic law, that is, the Fourier law;

$$\langle j \rangle = -\kappa \bigtriangledown T, \tag{1}$$

where κ is a thermal conductivity. It is well known that in integrable systems such as harmonic chains or ideal gas, the Fourier law is not valid since no temperature gradient is formed [1], while various numerical simulations of nonintegrable systems show temperature gradients. However, it is also found that thermal conductivity of nonintegrable systems such as the FPU chain diverge as N^α [2,3] where N is the degree of freedom. In other words, thermal conductivity becomes infinite in the thermodynamic limit.

On the other hand, finite conductivities are seen in some 1-D nonintegrable systems. Casati *et al.* invented so-called ding-a-ling model consisting of alternate harmonic oscilators and free particles, and found that the model has the finite conductivity [4]. The similar kind of the model which has finite conductivity is also investigated by Prosen and Robnik [5]. Most recently, Hu *et al.* found that the Frenkel-Kontrova model has the finite conductivity [6]. In these models, the conductivity converges at the certain value with relatively small N which does not exceed 100. This convergence makes apparent contrast with the FPU chain where the conductivity still grows even at $N \simeq 5000$ [2,7]. As the common feature of these systems which have finite conductivity, the external field is introduced to confine the movement of each particle. The Hamiltonian of the systems are represented as

$$H = \sum_i [\frac{p_i^2}{2m} + U(x_{i+1} - x_i) + V(x_i)], \tag{2}$$

where $V(x)$ is the external trapping potential. At this point, one might think that the external field plays the key role for obtaining the finite condutivity [6]. However, the finite condutivity is also obtained for the diatomic Toda lattice (DTL) [8] whose Hamiltonian is written as

$$H = \sum_i [\frac{p_i^2}{2m_i} + \exp(x_{i+1} - x_i)], \tag{3}$$

where m_i denotes the mass of alternate two different particles. The DTL has no external potential which is different from Eq.(2). It has been still under cover what is responsible for the finite conductivity.

Recently, Lepri *et al.* found that the autocorrelation function of the total heat current vanishes like $t^{-0.6}$ in the FPU chain [9]. This implies the divergence of the thermal conductivity as a result of the Green-Kubo formula;

$$\kappa = \lim_{t \to \infty} \lim_{V \to \infty} \frac{1}{V k_B T^2} \int_0^t dt' \langle J(0) J(t') \rangle, \tag{4}$$

where $J(t) = \int j(x,t)dx$, and V is the volume of the system.

Indeed, due to the conservation laws, long-time tails of the correlation functions are quite general results in fluids [10]. The rough explanation is as follows. Hydrodynamically, the local heat current $j(x,t)$ is expressed as

$$j(x,t) = h(x,t)v(x,t) - \kappa \bigtriangledown T(x,t), \tag{5}$$

where $h(x,t)$ and $v(x,t)$ denote local enthalpy density and local velocity of the fluid, respectively [11]. Since $v(x,t)$ appears in the first term of Eq.(5), an autocorrelation function of the total heat current $\langle J(0)J(t) \rangle$ includes effect of the velocity autocorrelation function (VACF) [12]. In the system where the total momentum preserves, asymptotic behavior of the VACF is propotional to $t^{-d/2}$, where d is the dimensionality of the system. Then $\langle J(0)J(t) \rangle$ also decays like $t^{-d/2}$, which implies the divergence of the integral of Eq. (4) for $d \le 2$. In the system where the total momentum does not preserve, the VACF vanishes much faster than that. For example, in the Lorentz gas the VACF decays like $-t^{-d/2-1}$ [13]. In those systems the VACF does not cause the divergence of Eq. (4). We remark that the contribution of the second term of Eq. (5) to $\langle J(0)J(t) \rangle$ is $t^{-d/2-1}$. This term is not responsible for the diverging conductivity.

Those explanations account for the diverging conductivity in the FPU chain, and also the finite ones of the models where the total momentum does not preserve due to the external field, such as the ding-a-ling model. However, the explanation does not apply to the diatomic

Toda lattice where the total momentum preserves. The fact that the DTL has a finite thermal conductivity has been invoking confusions. In this Rapid Communication, we recheck the result of Ref. [8] to find out what is really going on in the DTL.

The Hamiltonian of the DTL is given by Eq. (3). We perform numerical simulations of the DTL in contact with two thermal reservoirs whose temperatures are denoted as T_1 and T_2. Note that the choice of models for thermal reservoirs is critical, since there might exist the temperature gaps at the extrema of the lattice connecting with the reservoirs. It makes the definition of temperature gradient ambiguous, because the system will not obey the assigned boundary conditions; i.e. temperatures of the thermal reservoirs. Since thermal conductivity is defined as $\langle j \rangle / \bigtriangledown T$, it is important to determine $\bigtriangledown T$ exclusively by controll parameters. The model we adopt here is the thermal wall type [4,14]. When the particle collides with the wall, it reflects the particle back with a new momentum p at random. The probability distribution function of p is given by

$$\phi(p) = \frac{|p|}{mk_BT} \exp[-\frac{p^2}{2mk_BT}]. \tag{6}$$

The local heat flux $j_l(t)$ is defined as the energy transfer per unit time from the l-th particle to the (l+1)-th particle.

$$j_l(t) = \frac{\partial U(x_l - x_{l+1})}{\partial x_l} v_l. \tag{7}$$

The total heat current appearing in the Green-Kubo formula is

$$J(t) = \sum_{l=1}^{N} j_l(t)a, \tag{8}$$

where a is the average distance between two particles. The average current is then defined as

$$\langle j \rangle = \frac{1}{T} \int_0^T dt \frac{1}{aN} J(t). \tag{9}$$

Hereafter we fix the mass ratio of the particles to be 0.5, that is, $m_{2n-1} = 2m_{2n}$. The temperatures of the thermal reservoirs are set to be 100 and 10. Note that all these conditions are the same as Ref. [8] except for the reservoir model. Numerical integration is done by the symplectic integrator of the fourth-order [15] in order to preserve the symplectic structure of the phase space. Note that the distance between two thermal walls is aN so that the average density is fixed regardless of the number of particles. We set $a = 1$ and $m_{2n} = 1$ for nondimensionization.

First we check the temperature profile. We define the temperature of the l-th site as the long time average of $m_l v_l^2$ based on the virial theorem. The result is shown in Fig. 1. Since no gap is seen at the extrema, temperature

gradient $\bigtriangledown T$ becomes $(T_1 - T_2)/N$. We can safely define the thermal conductivity as

$$\kappa = \frac{\langle j \rangle N}{T_1 - T_2}, \tag{10}$$

where $\langle j \rangle$ is defined by Eq.(9). The system size dependence of the thermal conductivity is shown in Fig. 2. It is clearly seen that the conductivity diverges like $N^{0.35}$. The exponent 0.35 is very close to the one for the FPU chain (0.38). It is reasonable to consider that the origin of the divergence is the same as the case of the FPU chain, i.e. the long-time tail of the Green-Kubo integrand. We check an autocorrelation function of the total heat current $\langle J(0)J(t)\rangle$, by taking a periodic boundary condition instead of thermal walls. The initial condition is chosen within the microcanonical ensemble whose temperature is $(T_1 + T_2)/2 = 55$. Fig. 3 clearly shows the long-time tail which is approximately propotional to $t^{-0.65}$ just like the FPU chain. This long-time tail is the strong evidence for the diverging thermal conductivity in Fig. 2, and also helps the unified understanding of the heat conduction in 1-D lattices.

However, one may think that the temperature difference adopted here is so large that the linear response theory does not apply. To answer the suspicion, we check the thermal conductivity at the smaller temperature gradient which is closer to equilibrium, i.e. $T_1 = 5$, $T_2 = 4$. The system at this temperatures also shows the divergence of $N^{0.35}$ and the long-time tail of $t^{-0.65}$.

In order to confirm the divergence in the diatomic Toda lattice, we also test other versions of the DTL [16];

$$H = \sum_i \frac{p_i^2}{2m_i} + hardcore, \tag{11}$$

$$H = \sum_i [\frac{p_i^2}{2m_i} + \exp(x_i - x_{i+1}) + x_{i+1} - x_i]. \tag{12}$$

For thermal reservoirs, we use thermal wall model as before in the diatomic hard spheres of Eq. (11). Note that thermal reservoir employed in the simulation of Eq. (12) is the Langevin type.

$$m_1\dot{v}_1 + \zeta v_1 + \xi_1(t) = 1 - \exp(x_1 - x_2), \tag{13}$$
$$m_N\dot{v}_N + \zeta v_N + \xi_2(t) = -1 + \exp(x_{N-1} - x_N), \tag{14}$$

where $\xi_i(t)$ denotes the Gaussian white noise. ($\langle \xi_i(t) \rangle = 0$ and $\langle \xi_i(0)\xi_i(t) \rangle = 2\zeta k_B T_i \delta(t)$.) We set $T_1 = 5$ and $T_2 = 4$ for the both model. System size dependences of the thermal conductivity of these models are shown in Fig. 2. They also show the divergence of $N^{0.33} \sim N^{0.37}$.

The result obtained in this Rapid Communication is quite opposite to the results of Jackson *et al.* [8]. The keypoint is the formation of the temperature gradient. In Ref. [8], the temperature profile has large gaps at the extrema of the lattice so that the real temperature gradient gets smaller than $N/(T_1 - T_2)$. Hence it is improper to define the thermal conductivity as $\langle j \rangle N/(T_1 - T_2)$ as

they did. Moreover, since the size of the gap may depend on N, system size dependence of the thermal conductivity measured in that way is not precise.

The existence of the gaps is due to the model of the heat bath. In Ref. [8], the new momenta are randomly given to the end particles of the lattice. Although the distribution function is the same as ours, i.e. Eq. (6), the new momenta are given at finite time steps which is determined randomly from the uniform distribution. When the average time interval is shorter than the relaxation time of the lattice, the gap is formed. This issue has been partially reported in Refs. [5,7]. In our models, for instance, the Langevin model represented by Eqs. (13) and (14) yields temperature gaps when ζ becomes large.

In this Rapid Communication, we have confirmed that the thermal conductivity of the diatomic Toda lattice diverges as $N^{0.35}$ just like the FPU chain. This divergence is gereric in the 1-D momentum preserving systems, due to the long-time tails in the Green-Kubo integrands. Only are the systems where the total momentum does not preserve and the 3-D fluids expected to have the finite thermal condutivities in the thermodynamic limit.

However, it is still unclear that the quantitative conditions for the existence of temperature gradients, aside from the choice of the heat bath model. Nonintegrability itself is the necessary condition. Quantitative study of the transport processes from the viewpoint of dynamical systems must be the main focus of the future problem.

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FIG. 1. Temperature profile formed in the diatomic Toda lattice. The temperatures of the reservoirs are 100 and 10. System size N is 1000. The shape of the profile will not change with the increase of N.

FIG. 2. System size dependence of the thermal conductivity. Circles correspond to the diatomic Toda lattice with $T_1 = 100$, $T_2 = 10$. Squares denote diatomic hard spheres of Eq. (11). Triangles represent another version of the DTL written as Eq. (12). The solid line is propotional to $N^{0.35}$.

FIG. 3. The autocorrelation function of the total heat current with the periodic boundary condition. Dashed line is propotional to $t^{-0.65}$. System size N is 2000.